Hidden *d-wave Orbital Triplet* behind s± Superconductivity

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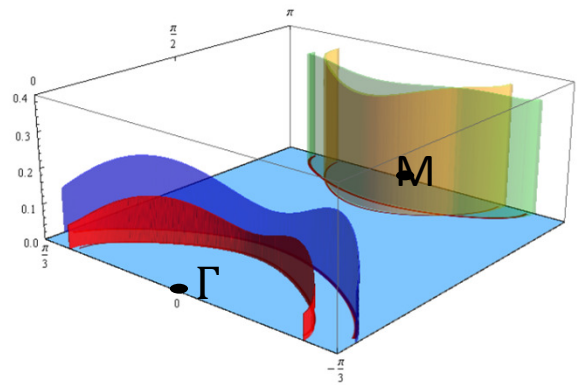
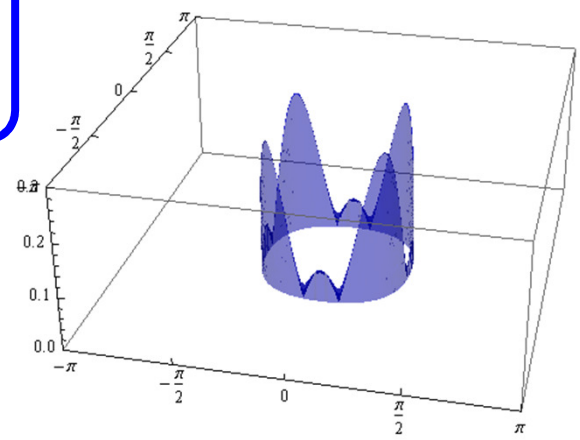
$\vec{L} + \vec{\alpha} = 0$



$s^{\pm}$ = d-wave orbital triplet!

$\vec{L} + \vec{\alpha} = 4$



T. Tzen Ong & P. Coleman, arXiv:1303.6325, T. Tzen Ong, P. Coleman & Joerg Schmalian, In preparation

Outline

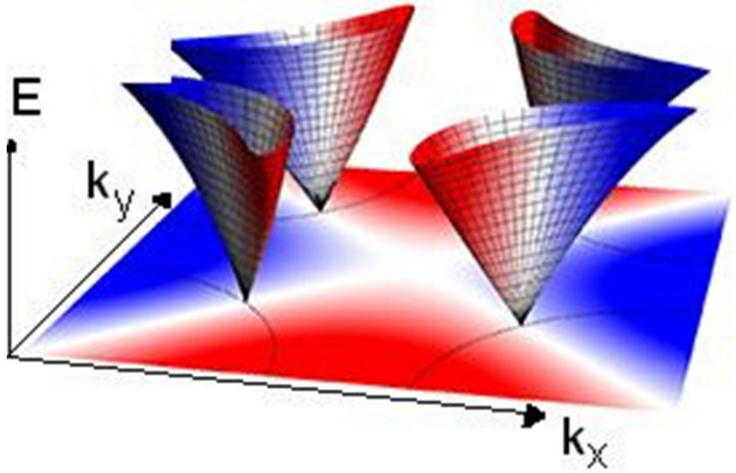
- Coulomb repulsion -> Higher angular momentum superconducting states
- ^{3}He-B with spin-orbit coupling
- Orbital helicity in Fe-SC band structure
- *Hidden d*-wave orbital triplet in Fe-based SCs

$$\boldsymbol{s^{\pm} = d - wave\ orbital\ triplet}$$

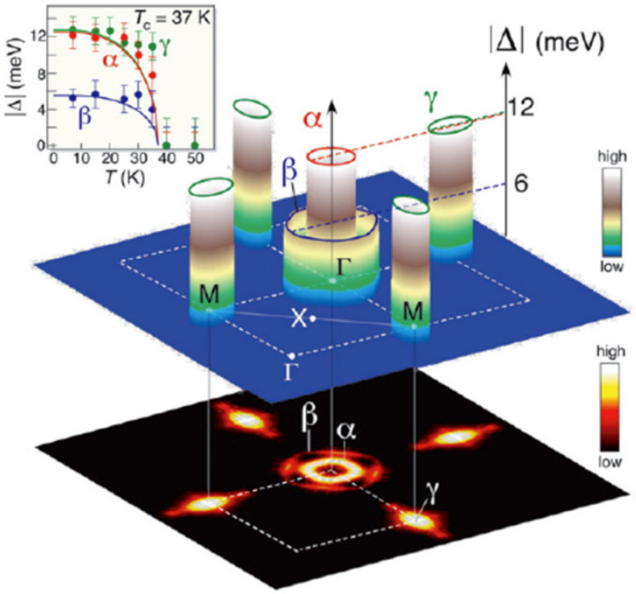
- Experimental consequences & Open Issues

Coulomb Repulsion & SC Order Parameter!

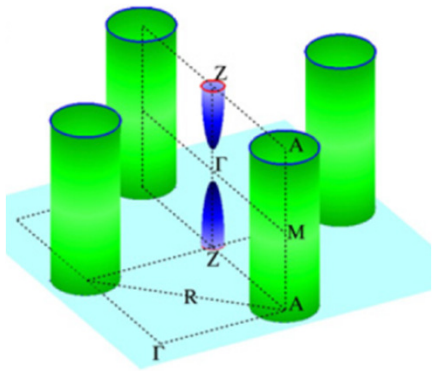
Cuprates



Fe-Based SCs



$Ba_{0.6}K_{0.4}Fe_2As_2$



FeSe

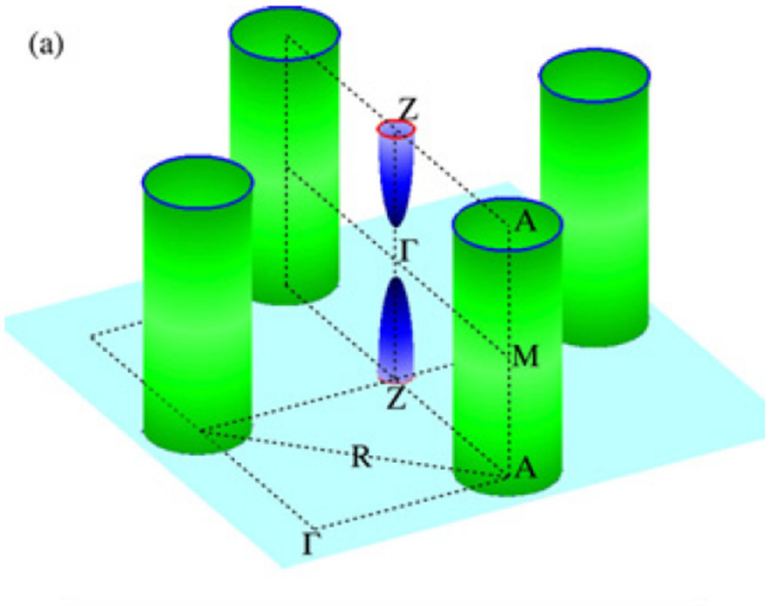
$$\langle \psi_\downarrow \psi_\uparrow \rangle = \int d\vec{k} \frac{\Delta_k}{2E_k} = 0$$

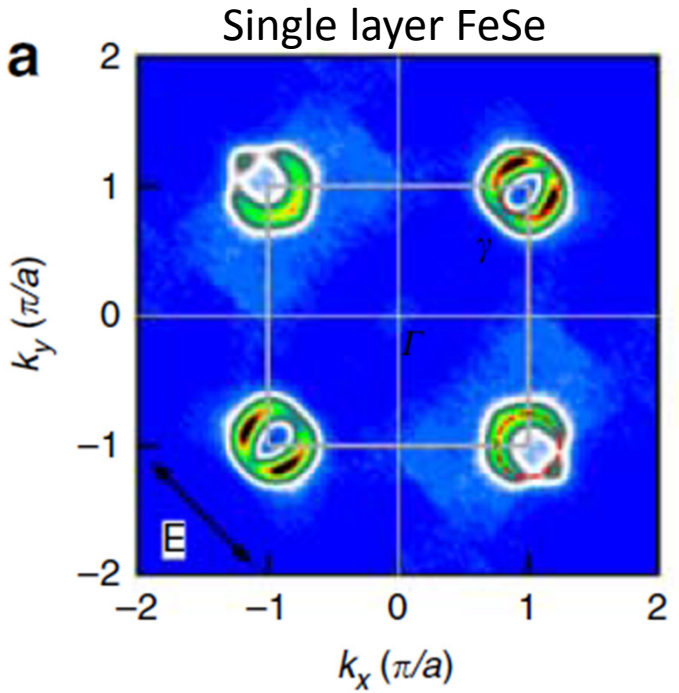
- Coulomb repulsion -> higher angular momentum SC states with nodes
  - Cuprates, ruthenates, heavy fermion SCs, *^{3}He-B*

Fe-SCs are exceptional ?

Fully Gapped State in Electron Pocket System

- Fully gapped SC state, T_c = 55K
- Electron pockets only.



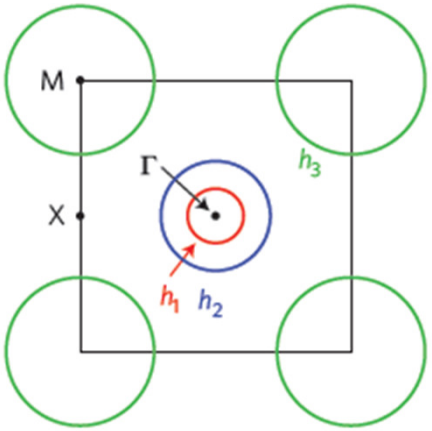


- ARPES shows an isotropic gap at Z
- Rules out d-wave superconducting order parameter!

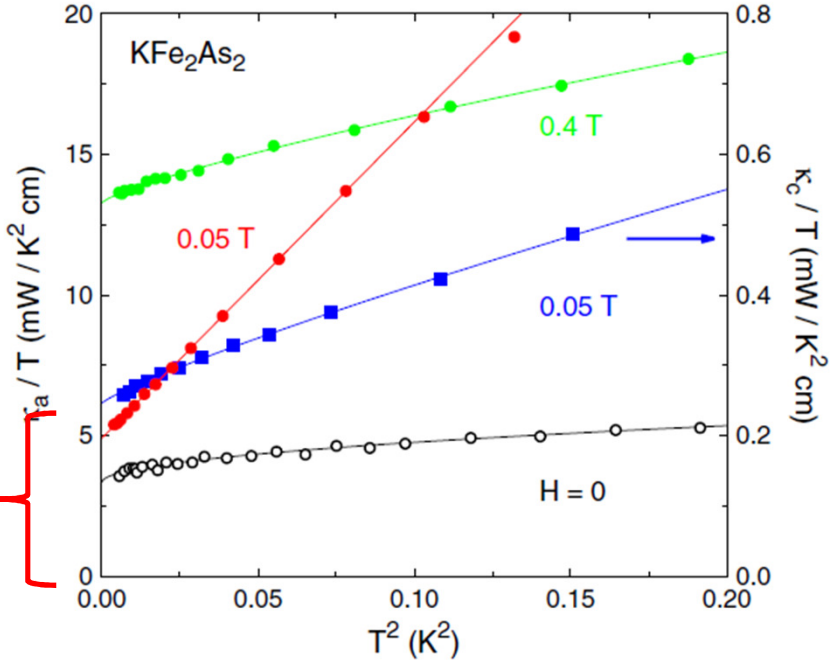
T. Qian and H. Ding *et. al.* PRL 106, 187001, (2011)
X.P. Wang and H. Ding *et. al.* EPL 99, 67001, (2012)

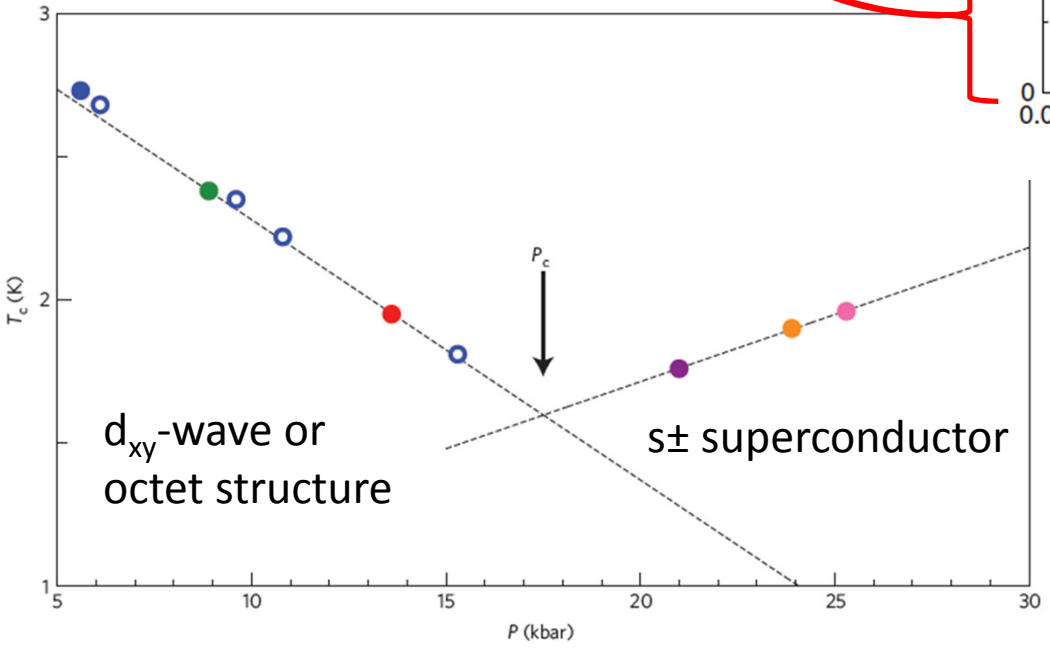
D. Liu *et. al.* Nat. Commun., 3, 931,(2012)

Lines Nodes in Hole-Doped KFe_2As_2



Finite thermal conductivity → Line nodes with nodal quasi-particles



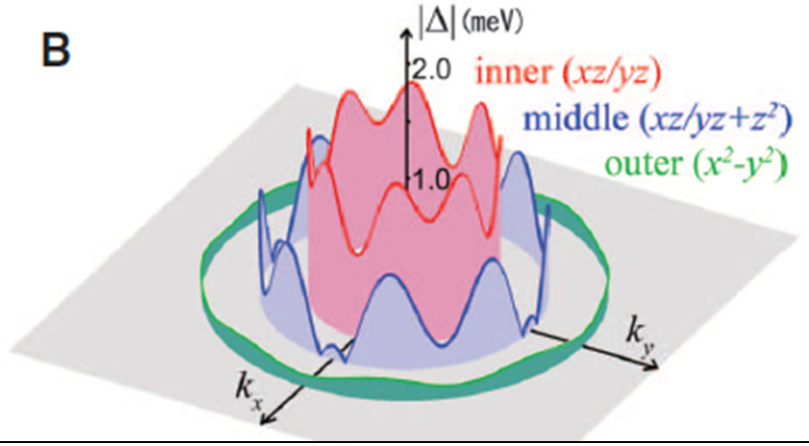


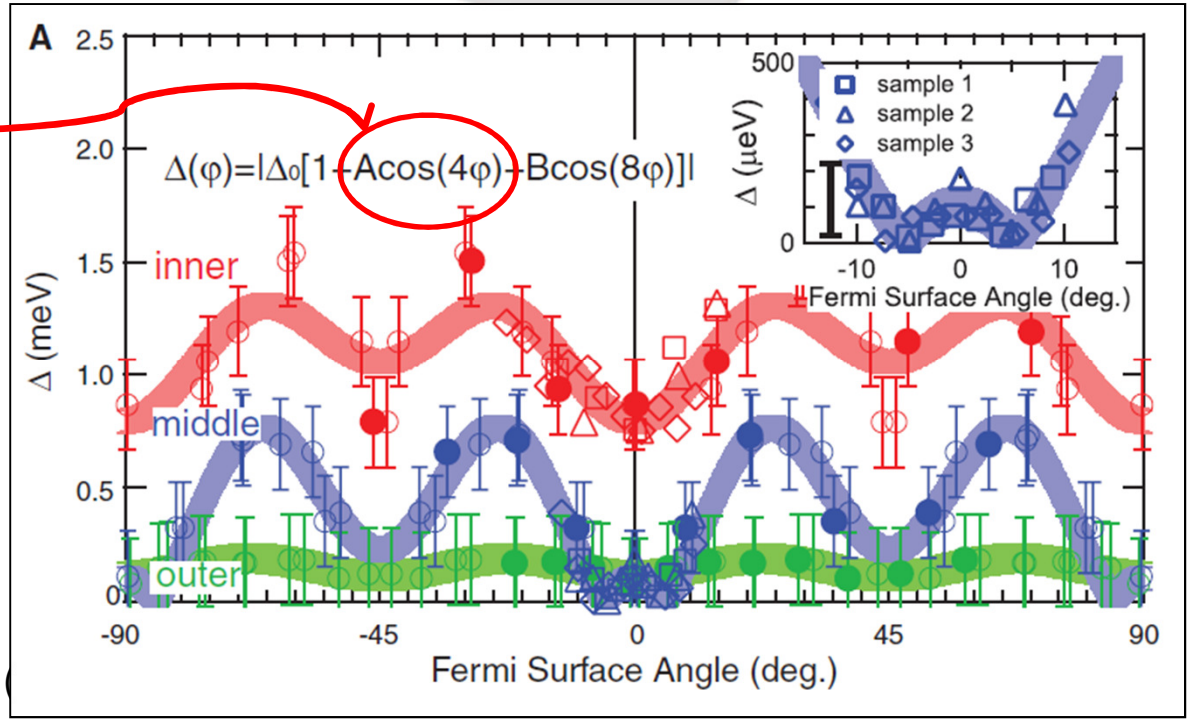
Reid, Taillefer *et. al.*, PRL **109**, 087001, (2012)
Tafti, Taillefer *et. al.*, Nat. Phys. **9**, 349 (2013)

Naturally implies d-wave state

Octet Structure in Hole-Doped KFe_2As_2

- Competition between s-wave and d-wave?
- Or higher angular momentum SC state → **Octet structure** from ARPES!

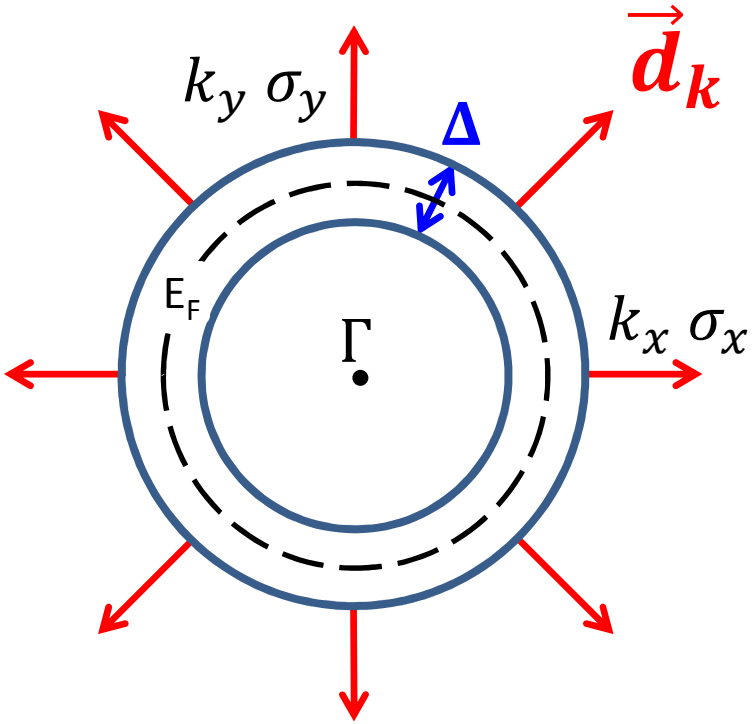




Okazaki, Shin *et. al.*, Science 337, **1314** (

^{3}He-B

$$H^{sc} = \sum_k \Delta\, c^{\dagger}_{k,\alpha} \left(\left(k_x\, \sigma_x + k_y \sigma_y \right) i\sigma_2 \right)_{\alpha\beta} c^{\dagger}_{-k,\beta}$$



Fully-gapped *p*-wave superfluid and minimizes on-site repulsion!

Superfluid O.P rotates in *k*-space:

$$\vec{d}_k = \begin{pmatrix} k_x \\ k_y \end{pmatrix}$$

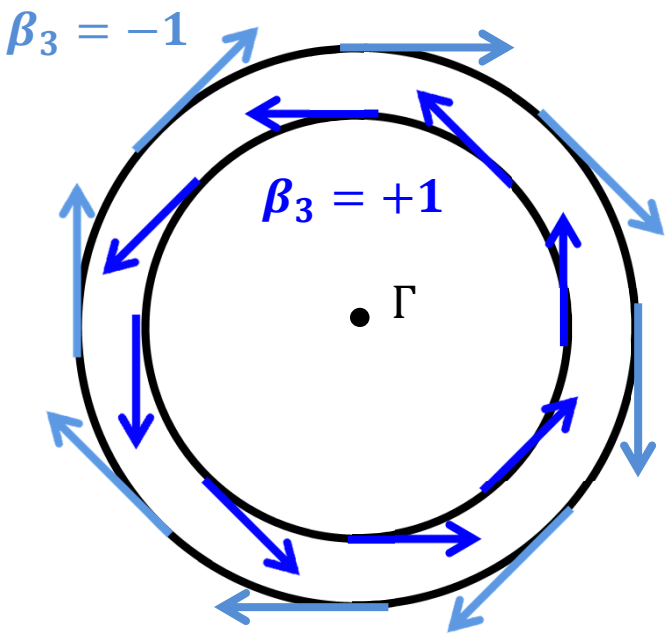
Topological invariant:

$$\nu = \int \frac{dk}{2\pi} \vec{d}_k \times \nabla\, \vec{d}_k = 1$$

Spin-Orbit Coupling

$$\mathrm{H}^{so} = \sum_k c_k^{\dagger}\, v\, \underbrace{\left(\hat{z} \times \vec{k}\right)} \cdot \vec{\sigma} c_k$$

$\vec{n}_k$: **Helicity vector**



- Helical basis, $\beta_3 = \vec{n}_k \cdot \vec{\sigma} = \pm 1$
- Spin-orbit field couples orbital angular momentum and spin
  - $J = L + S$

^{3}He-B with Spin-Orbit Coupling

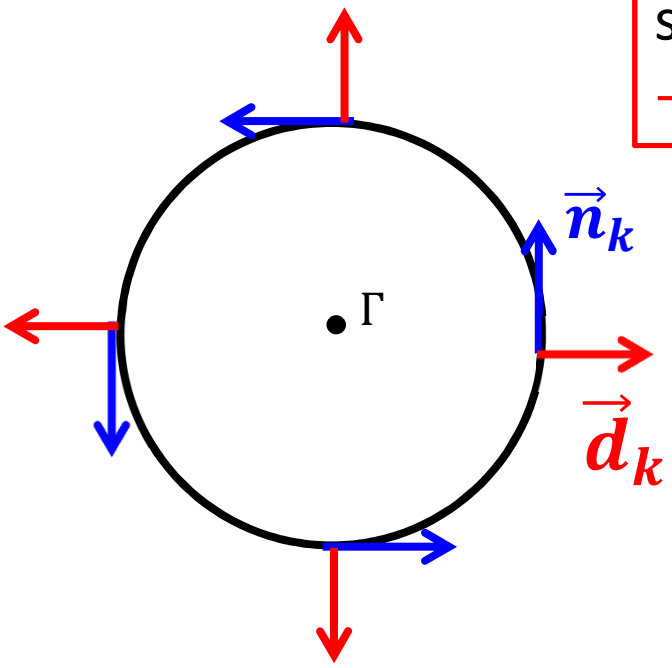
$$\mathrm{H}^{so} = \sum_k c_k^\dagger \, v \left(\hat{z} \times \vec{k}\right) \cdot \vec{\sigma} c_k \qquad \mathrm{H}^{sc} = \sum_k c_{k\alpha}^\dagger \, \Delta \, \underbrace{\vec{d}_k \cdot \vec{\sigma}_{\alpha\beta}}_{\vec{d}_k} c_{-k\beta}^\dagger + H.C.$$

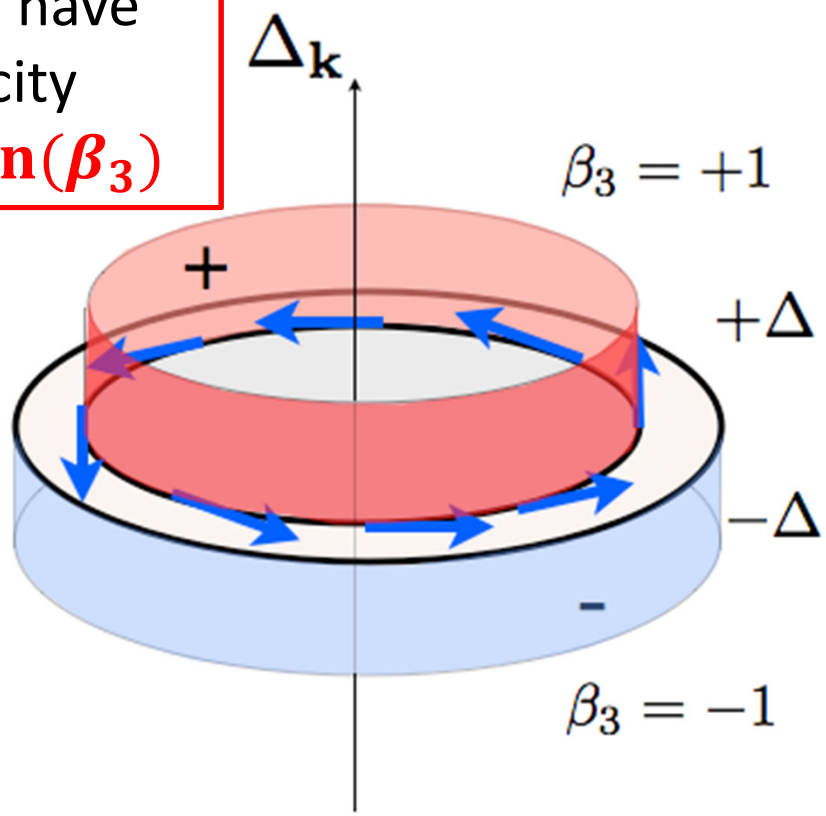
Spin-orbit field couples $L + S$ $\boldsymbol{\vec{d}_k}$

$\boldsymbol{J = L + S = 0}$

$\vec{n}_k$ and $\vec{d}_k$ have same helicity

$\rightarrow \boldsymbol{\Delta = \mathrm{sgn}(\beta_3)}$

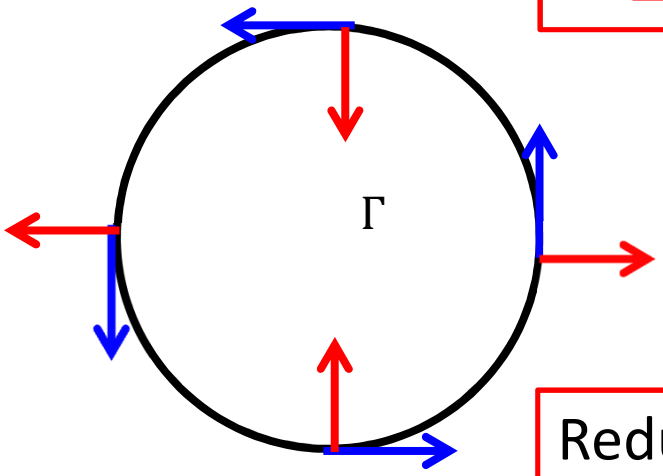


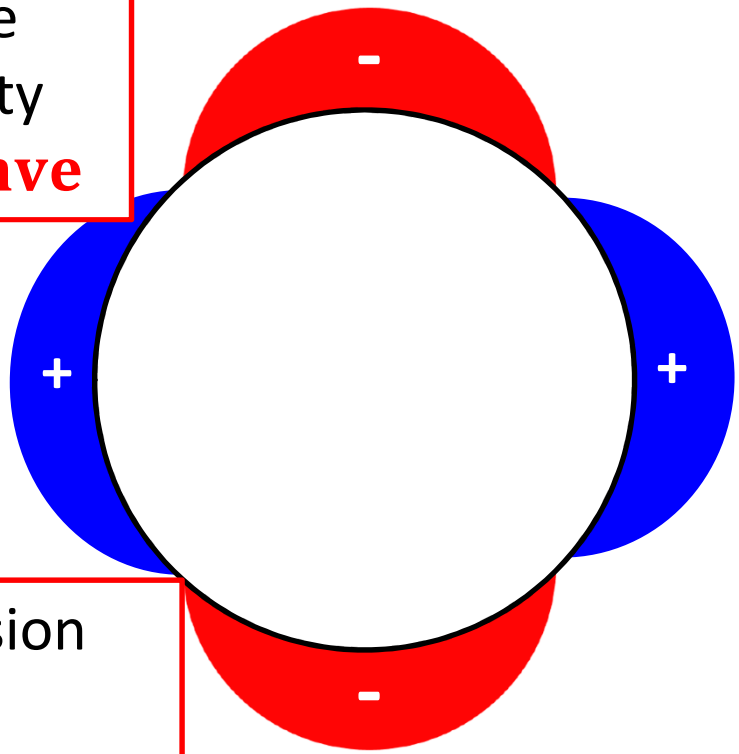


$\boldsymbol{J = L + S = 2}$

$\vec{n}_k$ and $\vec{d}_k$ have opposite helicity

$\rightarrow \boldsymbol{\Delta = d - wave}$





Reduces repulsion @ cost of condensation energy

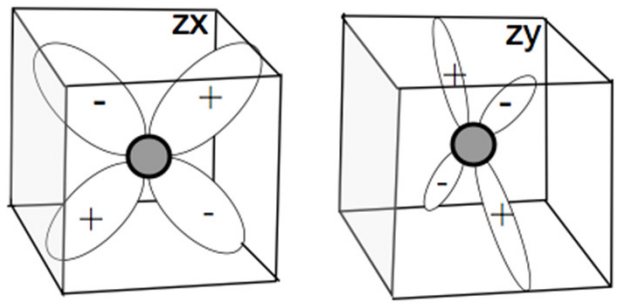
Outline

- ✓ Coulomb repulsion -> Higher angular momentum superconducting states
  - Are Fe-based SCs an exception?
- ✓ ^{3}He-B with spin-orbit coupling
  - $L + S = 0 \rightarrow$ s± in helical basis
  - $L + S = 2 \rightarrow$ *d-wave* in helical basis

- **Orbital helicity in Fe-SC band structure**
- ***Hidden d*-wave orbital triplet in Fe-based SCs**
  - $L + \alpha = 0 \rightarrow$ low-spin s± state
  - $L + \alpha = 4 \rightarrow$ high-spin octet state
  - QPT from low-spin to high-spin SC state?
- Experimental consequences & Open Issues

Internal Orbital Iso-Spin

- Crystalline Symmetry – Introduces new **internal** orbital iso-spin degrees of freedom ($\vec{\alpha}$)



$$c_{k\sigma} \rightarrow c_{k\alpha\sigma}$$

Orbital Rashba coupling :

Inter-orbital hopping leads to coupling between kinetic orbital motion and internal orbital iso-spin

Orbital Rashba Field

- **Orbital Rashba field :** Coupling between kinetic angular momentum ($\vec{L}$) and atomic orbital iso-spin ($\vec{\alpha}$).

  $-\vec{J} = \vec{L} + \vec{\alpha}$

  – analogous to spin-orbit Rashba coupling.

- Kinetic Hamiltonian:

$$H^0 = \sum_k c^\dagger_{k,\alpha,\sigma}\left(\epsilon_s(k)\mathbf{1} + \vec{B}_k \cdot \vec{\alpha}\right)c_{k,\alpha',\sigma}$$

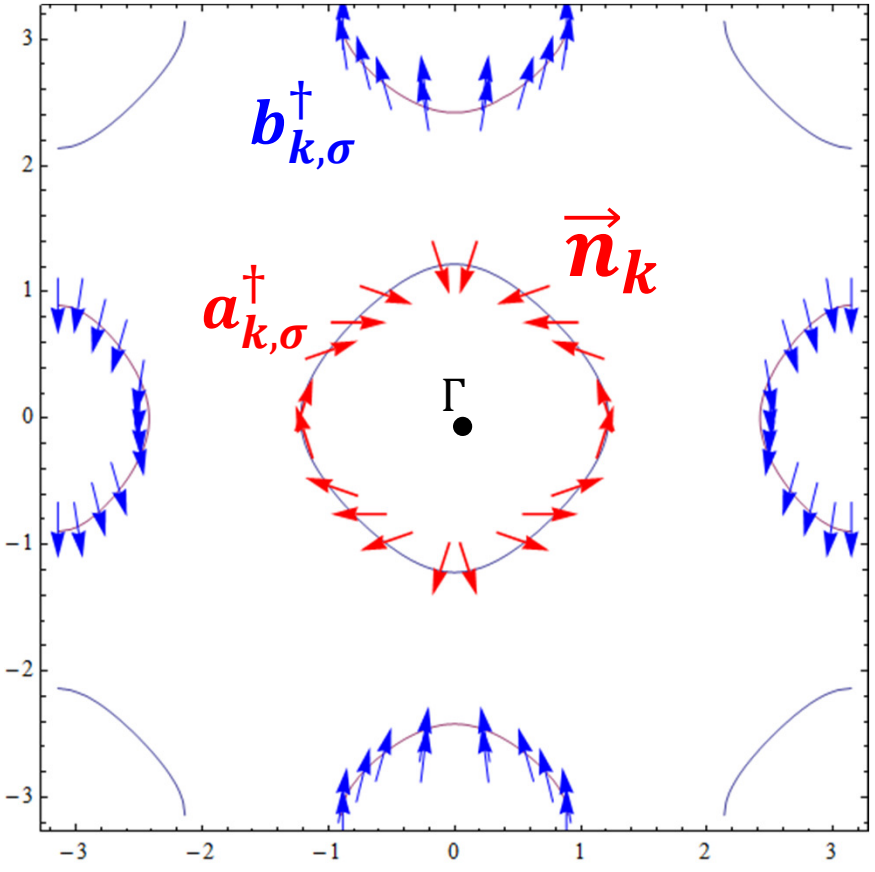
- $\vec{B}_k = \left[\epsilon_{xy}(k), 0, \epsilon_{x^2-y^2}(k)\right] \equiv B_k \underbrace{\vec{n}_k}_{\textit{Helicity vector}}$

- Pauli matrices in orbital iso-spin space, $\vec{\alpha}$

Orbital Helicity

$$\mathbf{E_k} = \epsilon_s(k) + sgn(\alpha)B_k$$

- Orbital helical basis. Hole pocket: $\alpha = -1$, Electron pockets: $\alpha = +1$
  - Hole and electron pocket quasi-particles, $a_{k\sigma}$ and $b_{k\sigma}$.



- Quasi-particles: linear superposition of xz and yz orbitals.
- $a_{k\sigma} = u_k\, c_{k,\,xz,\sigma} + v_k\, c_{k,\,yz,\sigma}$
- $b_{k\sigma} = u_k\, c_{k,\,yz,\sigma} - v_k\, c_{k,\,xz,\sigma}$

Ran, Lee *et. al.*, PRB **79**, 014505 (2009)

$s^{\pm}$ Superconductivity in Band Basis

- $H^{sc} = \Delta \sum_k a^{\dagger}_{k\uparrow} a^{\dagger}_{-k\downarrow} - b^{\dagger}_{k\uparrow} b^{\dagger}_{-k\downarrow} + H.C.$
  - $a_{k\sigma} = u_k \, c_{k,\,xz,\sigma} + v_k \, c_{k,\,yz,\sigma}$
  - $b_{k\sigma} = u_k \, c_{k,\,yz,\sigma} - v_k \, c_{k,\,xz,\sigma}$
  - Quasi-particles coherence factors, u_k and v_k have d-wave form factors

Orbital Basis = d-wave Orbital Triplet!

- $H^{sc} = \Delta \sum_k c^{\dagger}_{k\,\alpha\uparrow} \left((u_k^2 - v_k^2)\alpha_3 + 2\, u_k v_k \alpha_1 \right) c^{\dagger}_{-k\,\alpha'\downarrow} + \text{H.C.}$

$$= \frac{1}{2} \sum_k \boldsymbol{c^{\dagger}_{k\,\alpha\,\sigma}} \left(\boldsymbol{\Delta_{x^2-y^2}\ \alpha_3 + \Delta_{xy}\ \alpha_1} \right) (\boldsymbol{i\sigma_2}) \boldsymbol{c^{\dagger}_{-k\,\alpha'\sigma'}} + \text{H.C.}$$

$s^{\pm}$ = d-wave Orbital Triplet!

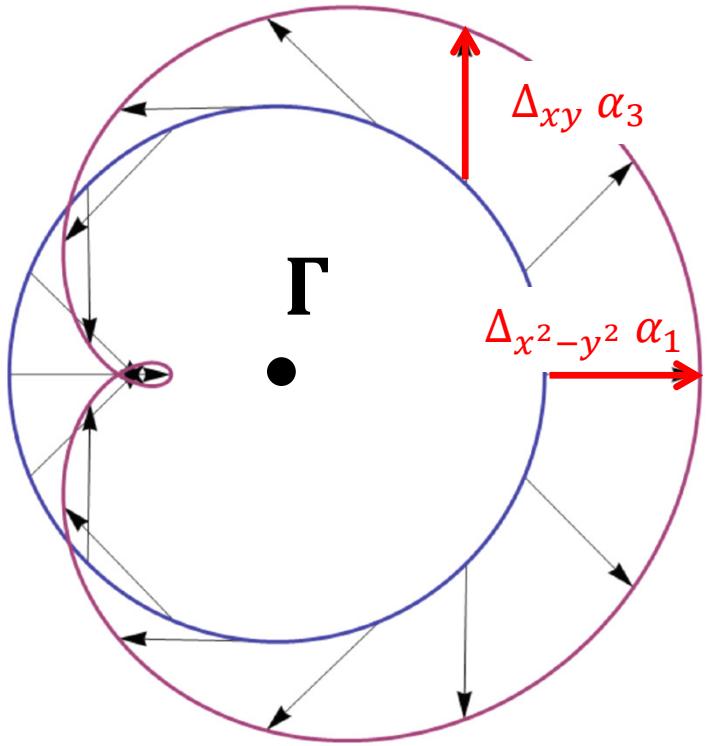
Orbital Triplet Superconductivity with Orbital Rashba Coupling

$$H = \sum_{k} \psi^{\dagger}_{k,\alpha,\sigma}\left(\epsilon_s(k)1\,\gamma_3 + \vec{B}_k \cdot \vec{\alpha} + \vec{d}_k \cdot \vec{\alpha}\,\gamma_1\right)\psi_{k,\alpha',\sigma}$$

Superconducting $\vec{d}_k$-vector:

$$\vec{d}_k \equiv \begin{pmatrix} -\Delta_{x^2-y^2} \\ 0 \\ \Delta_{xy} \end{pmatrix}$$

$\vec{d}_k$ *vector*

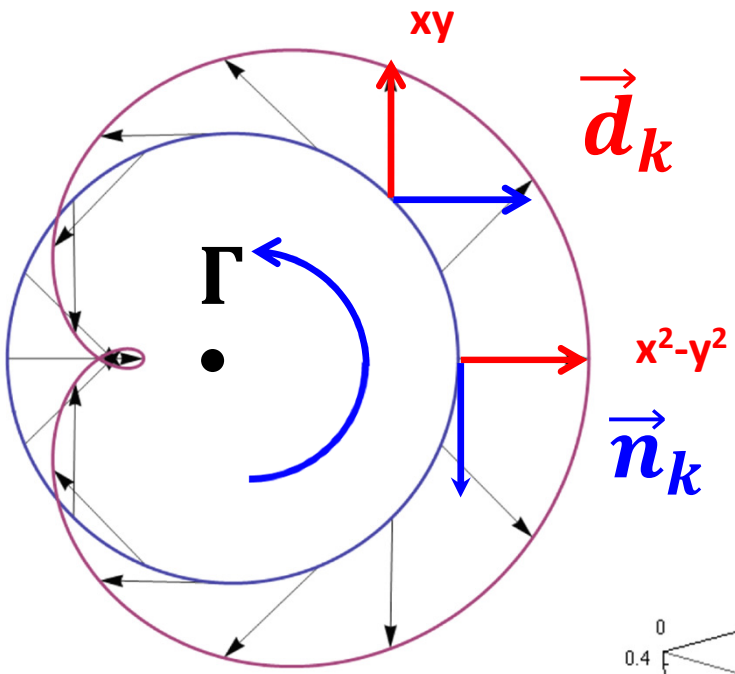


Helicity: $\int \frac{d\vec{k}}{2\pi}\vec{d}_k \times \nabla_{\mathbf{k}}\,\vec{d}_k \equiv \nu = \pm 2$

- Balian-Werthammer spinor:

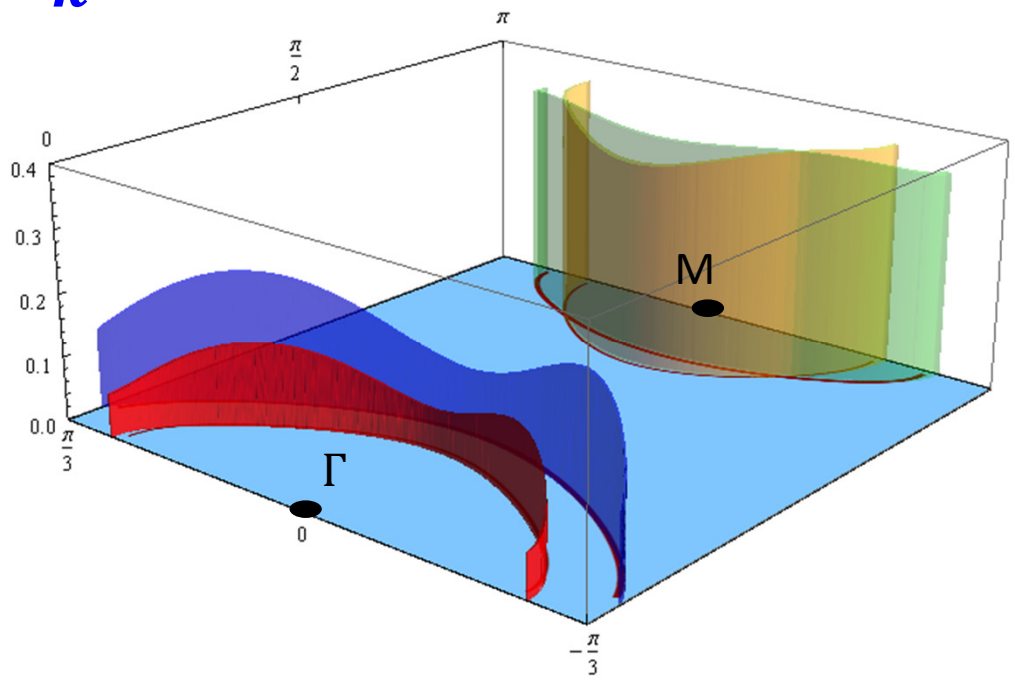
$$\psi_{k,\alpha,\sigma} \equiv \left[c_{k,\alpha,\sigma}, (i\alpha_2 i\sigma_2)c^{\dagger}_{k,\alpha,\sigma}\right]^T$$

In-Phase Rotation = $s^{\pm}$ Superconductivity



- $\vec{J} = \vec{L} + \vec{\alpha} = 0$
- Low angular momentum state = **s±**

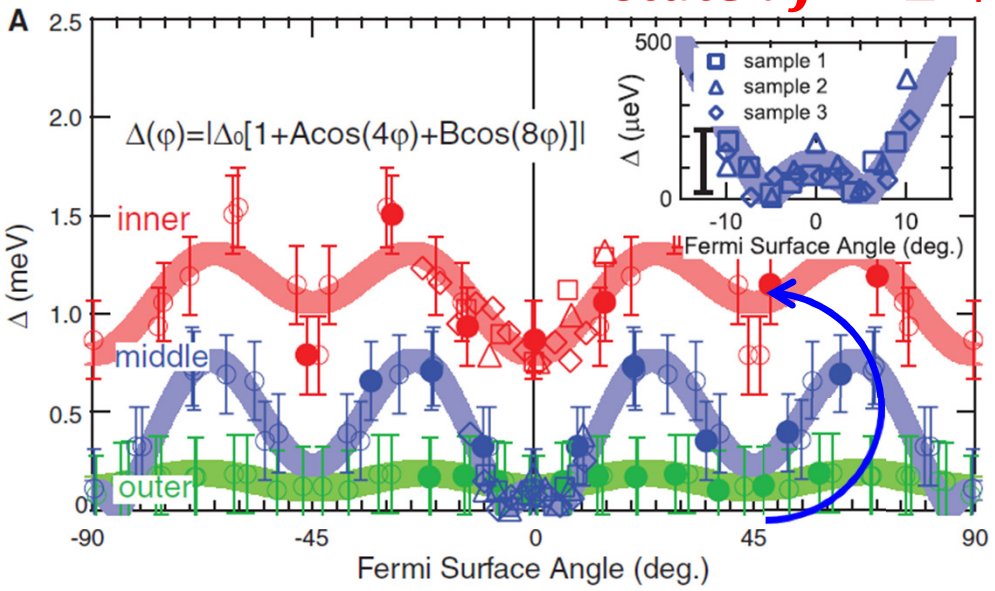
$\nu = +2$



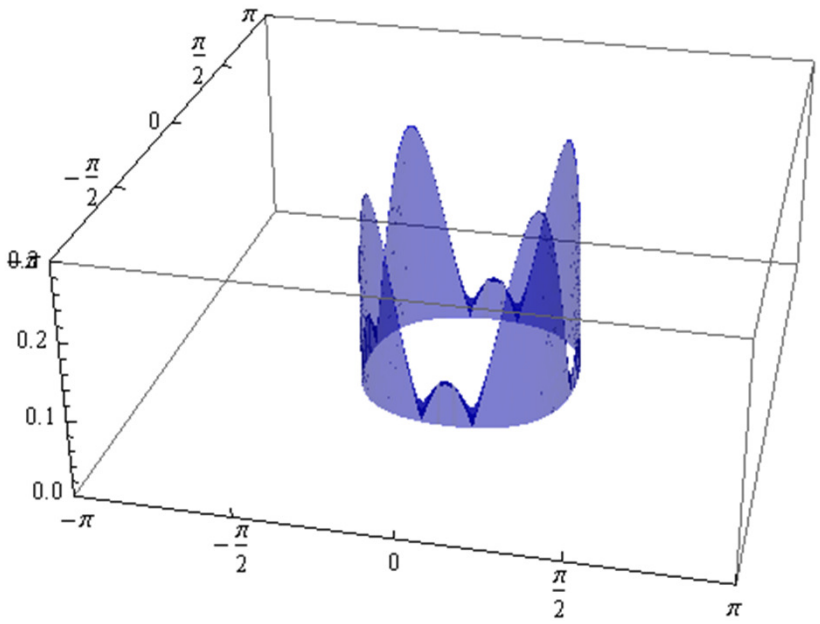
Octet Structure in KFe_2As_2

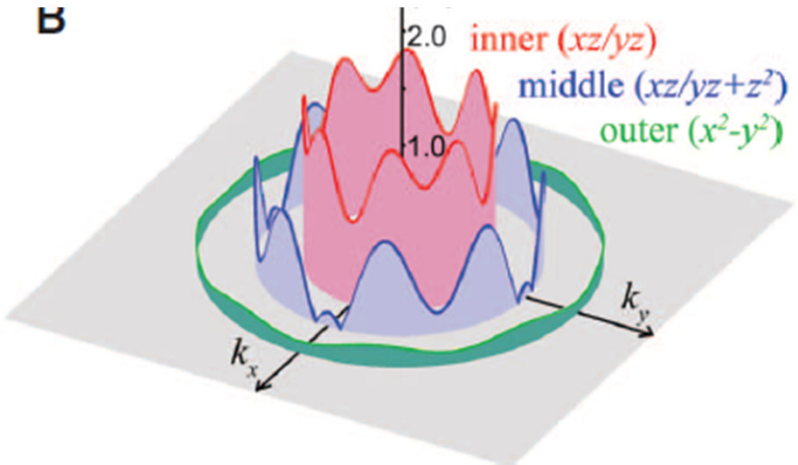
$\vec{d}_k$ *and* $\vec{n}_k$ *out-of-phase -> High angular momentum SC*

state : $\vec{J} = \vec{L} + \vec{\alpha} = 4$



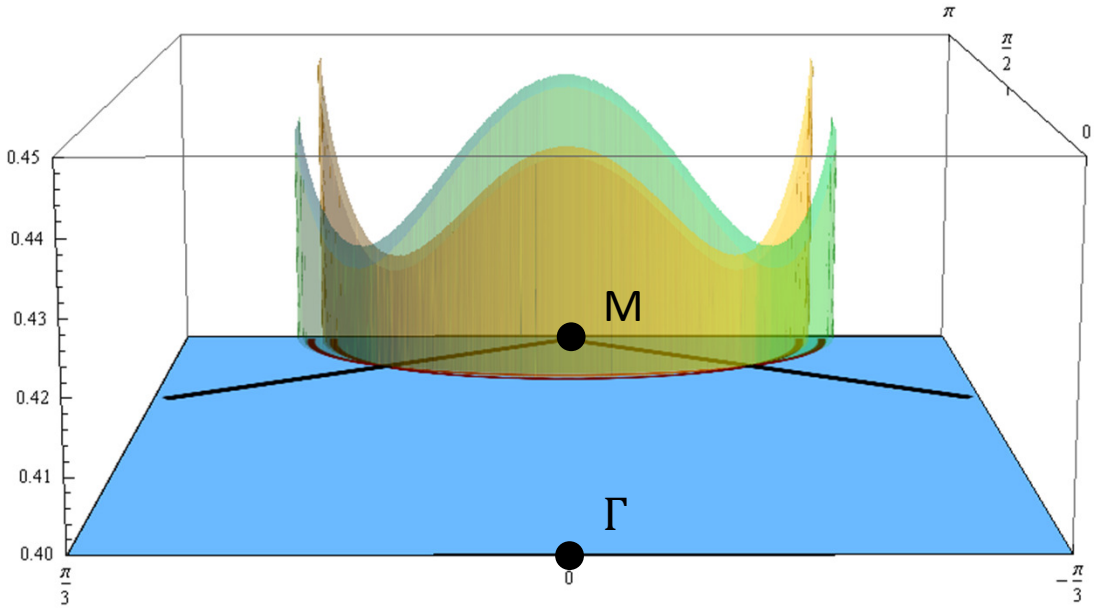
$\Delta \sim Cos4\theta$



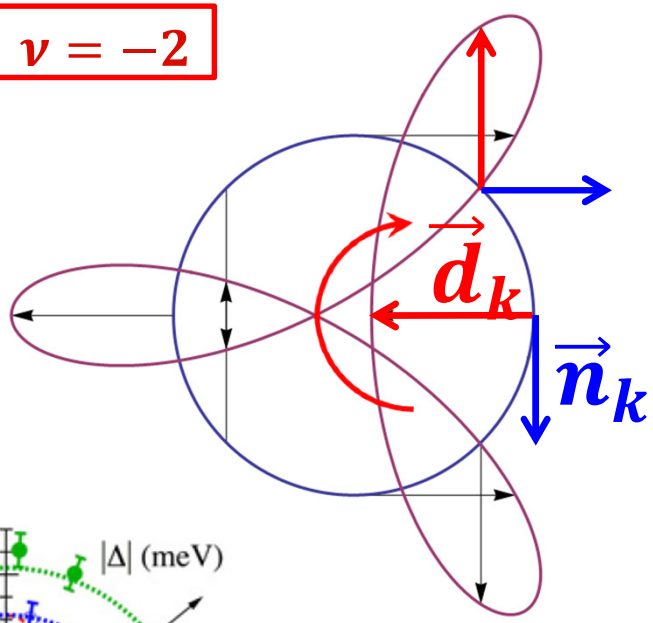


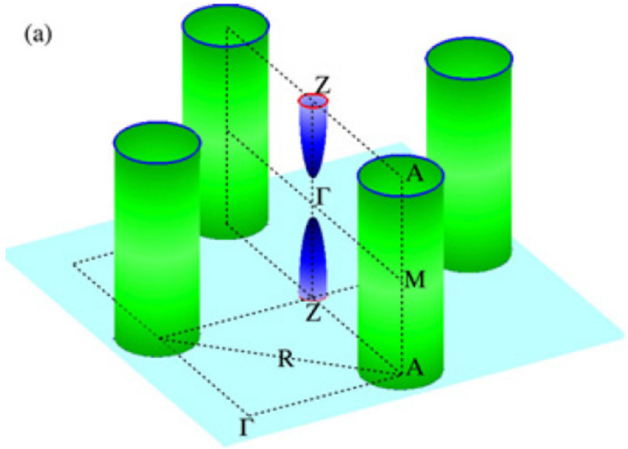
Okazaki, Shin *et. al.*, Science 337, **1314** (2012)

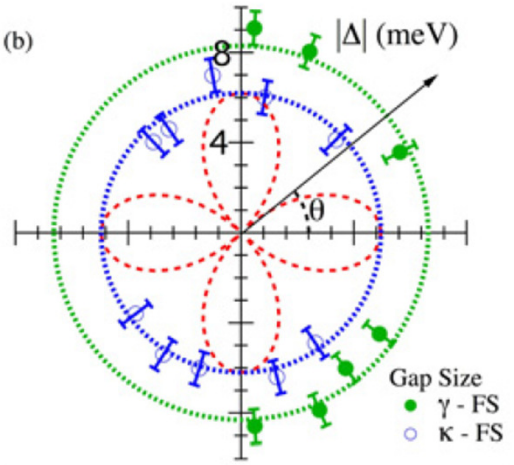
Electron Pocket System



$\nu = -2$



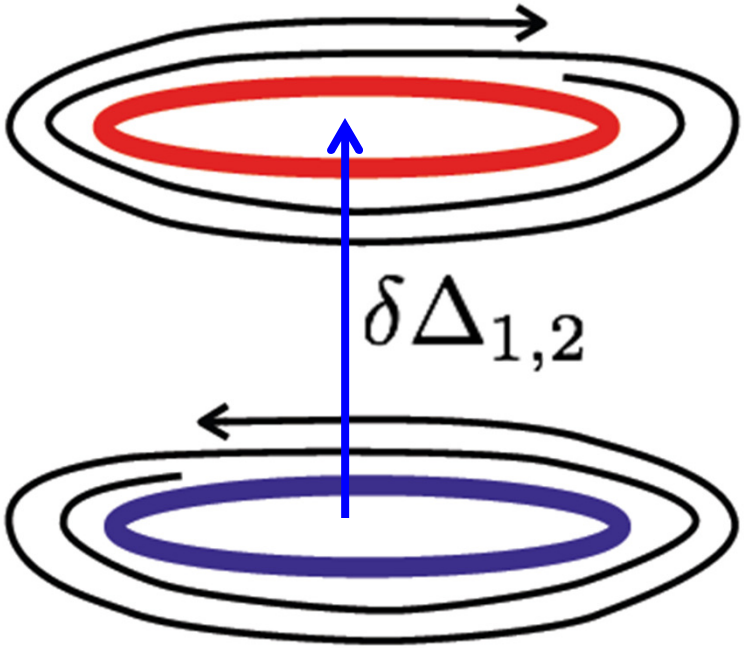




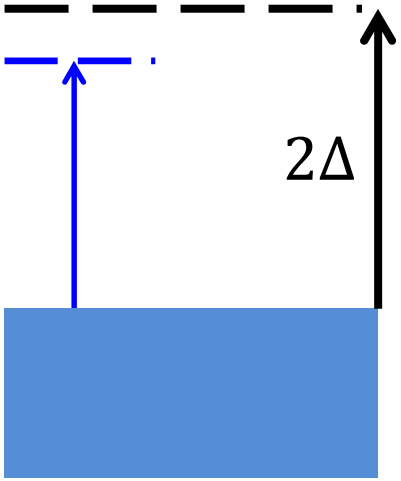
t0 = 1.0, t1 = 0.15, t3 = 0.7, t4 = 0.7, μ = -4.0, Δ_{xy} = 0.5, Δ_{x2-y2} = -0.25

Raman Active Modes

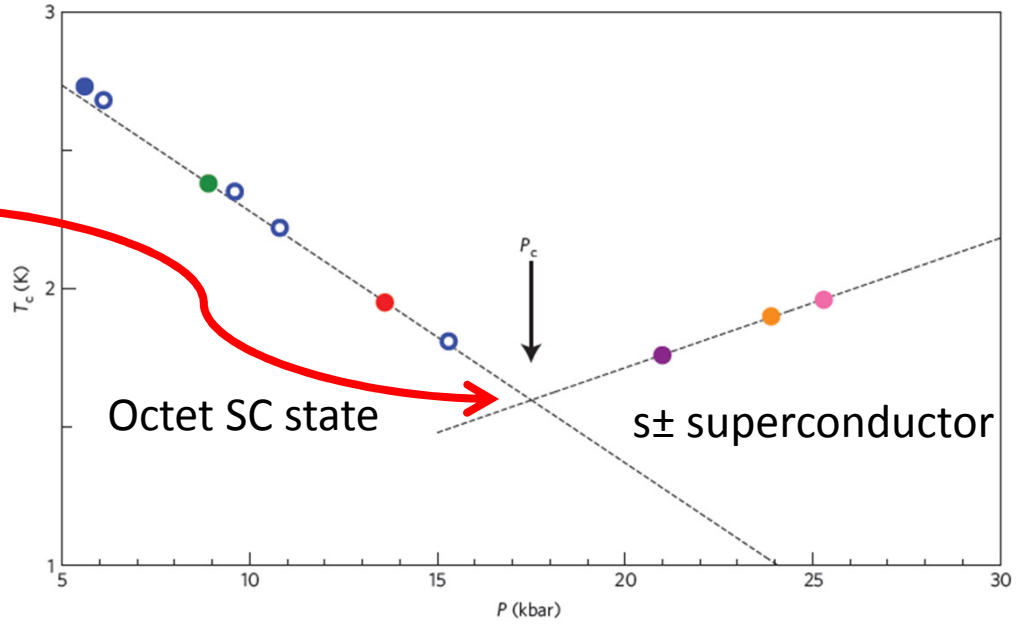
Excited Cooper pairs with reverse chirality



A_{1g} Leggett mode

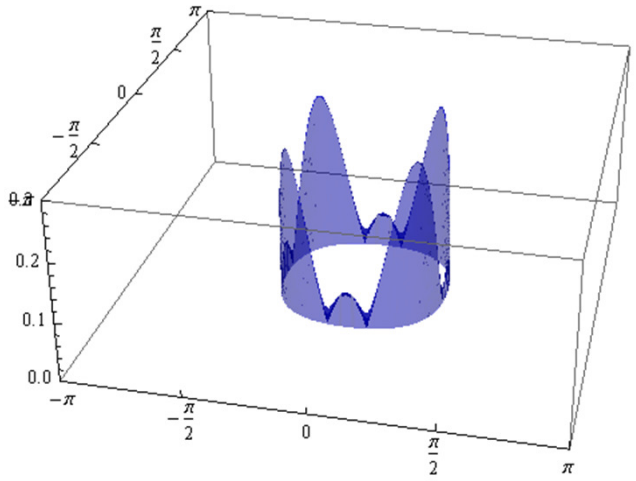


- **Gapless Leggett mode at QPT between low-spin and high-spin SC state!**

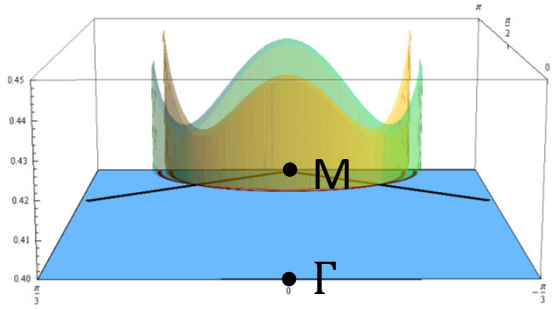


Conclusion

- $s^{\pm}$ = ***d-wave* orbital triplet** SC state
  - Orbital helicity of band structure
- Low-spin state = Fully gapped $s^{\pm}$ SC states
- High-spin state
  - Fully gapped state in el-system
  - Octet SC gap in hole systems



- Experimental consequences
  - Raman active modes
  - Gapless Leggett mode at QPT
  - Topological invariant of *d*-vector



T. Tzen Ong & P. Coleman, arXiv:1303.6325
T. Tzen Ong, P. Coleman & Joerg Schmalian, In preparation